Using Monte Carlo Simulation to derive Electron Energy Distribution Functions in Argon Plasma

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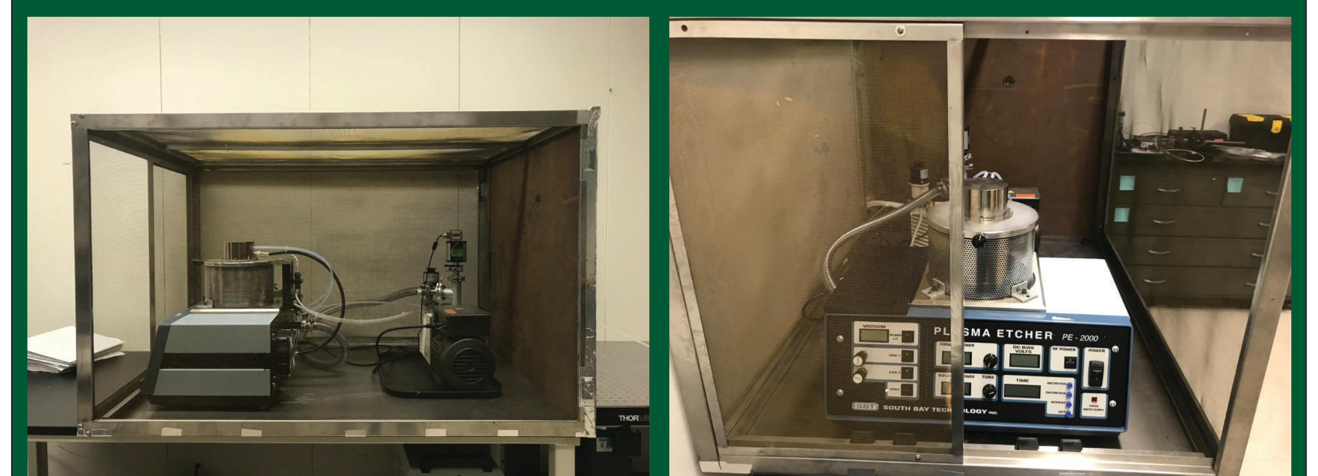
Introduction

Over the past handfull of decades the semiconductor industry has consistently miniturized computer chips but in recent times seems to have hit their limit. The process of using high-speed plasma discharges to create these integraded circuits is known as plasma etching. By studying the properties of plasma, one can hope to be able to improve plasma etching process.

In our study we simulated a low-temperature argon plasma produced by heating argon gas with radio-frequency (RF) electromagnetic (EM) waves. Simulated electrons were propagated throughout the plasma and experienced both elastic and inelastic collisions including ionization and quantum excitation.

Images of plasma etching system within Faraday Cage shown below, he hope to improve results from hands on experiements by simulating electron collisions within plasma using a Monte Carlo Simulation Python script.



Theory

Collision Frequencies

Collision Probability derived from cross section σ(E)

$$f = N_A \sigma(E)\sqrt{\frac{2E}{m_e}}$$

- N_A is population density in units of atoms per cube meter
- σ(E) is cross section for a collision at energy E
- m_e is mass of an electron

Null Collision Frequency

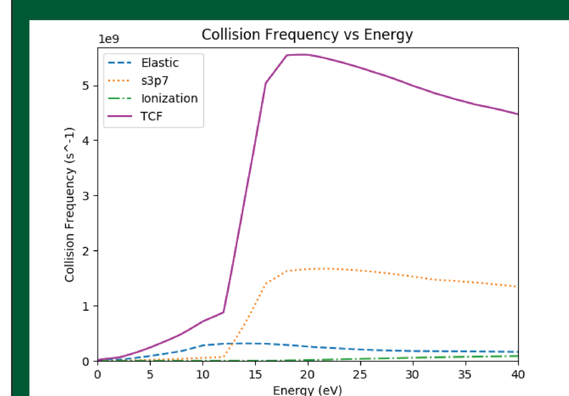
$$f_{null}(\varepsilon) = Max[f_{total}(\varepsilon)] - f_{total}(\varepsilon)$$

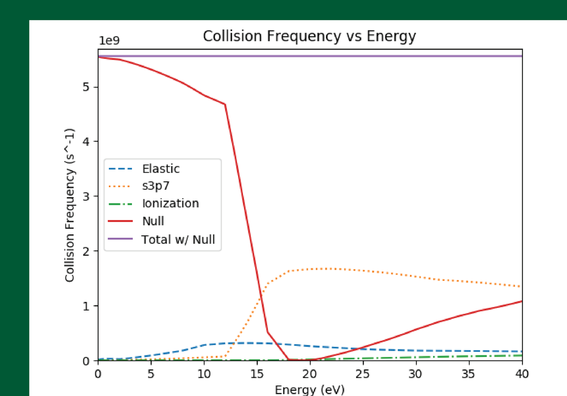
- f_{null} is the collision frequency corresponding to no collision
- $Max[f_{total}(E)]$ is the maximum total collsion frequency
- $f_{total}(E)$ is the total collision frequency at the current energy

Timestep

- Derived from time of flight
- Exception made for energys below 0.01 due to 1/TCF factor

$$E > 0.01eV : dt = \frac{-\log(1-r)}{TCF}$$
$$E <= 0.01eV : dt = 10^{-7}s$$





Collision Theory

Equations of motion from Newton's 2nd Law

$$F_x = q_e E_x = m_e a_x \rightarrow a_x = (q_e E)/m_e \qquad x = x_0 + v_{0x}t + \frac{1}{2}a_x t^2$$

- F_x is the x-component of the electric force
- a_x is the acceleration the electron experiences
- q_e the charge of an electron

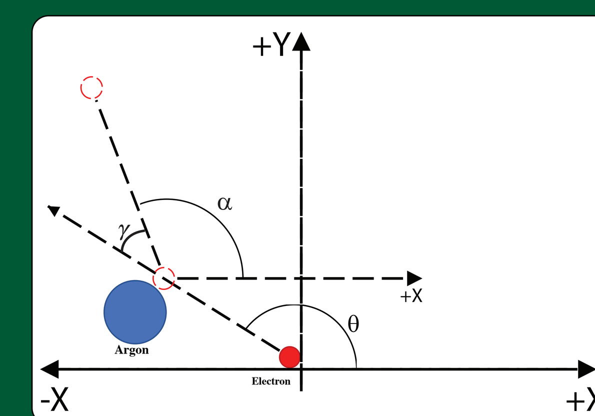
Conservation of Energy and Momentum

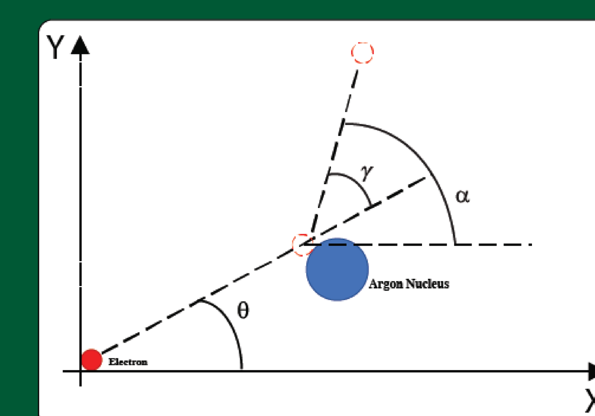
$$\tan\alpha = \tan(\theta+\gamma)$$

$$v_a = \frac{(v_{ix} + v_{iy}\tan\alpha)\frac{1}{\sqrt{1+\tan^2\alpha}} \pm \sqrt{(v_{ix} + v_{iy}\tan\alpha)^2\frac{1}{1+\tan^2\alpha} - \frac{2\Delta E}{m_a}(1+\frac{m_a}{m_e})}}{1+\frac{m_a}{m_e}}$$

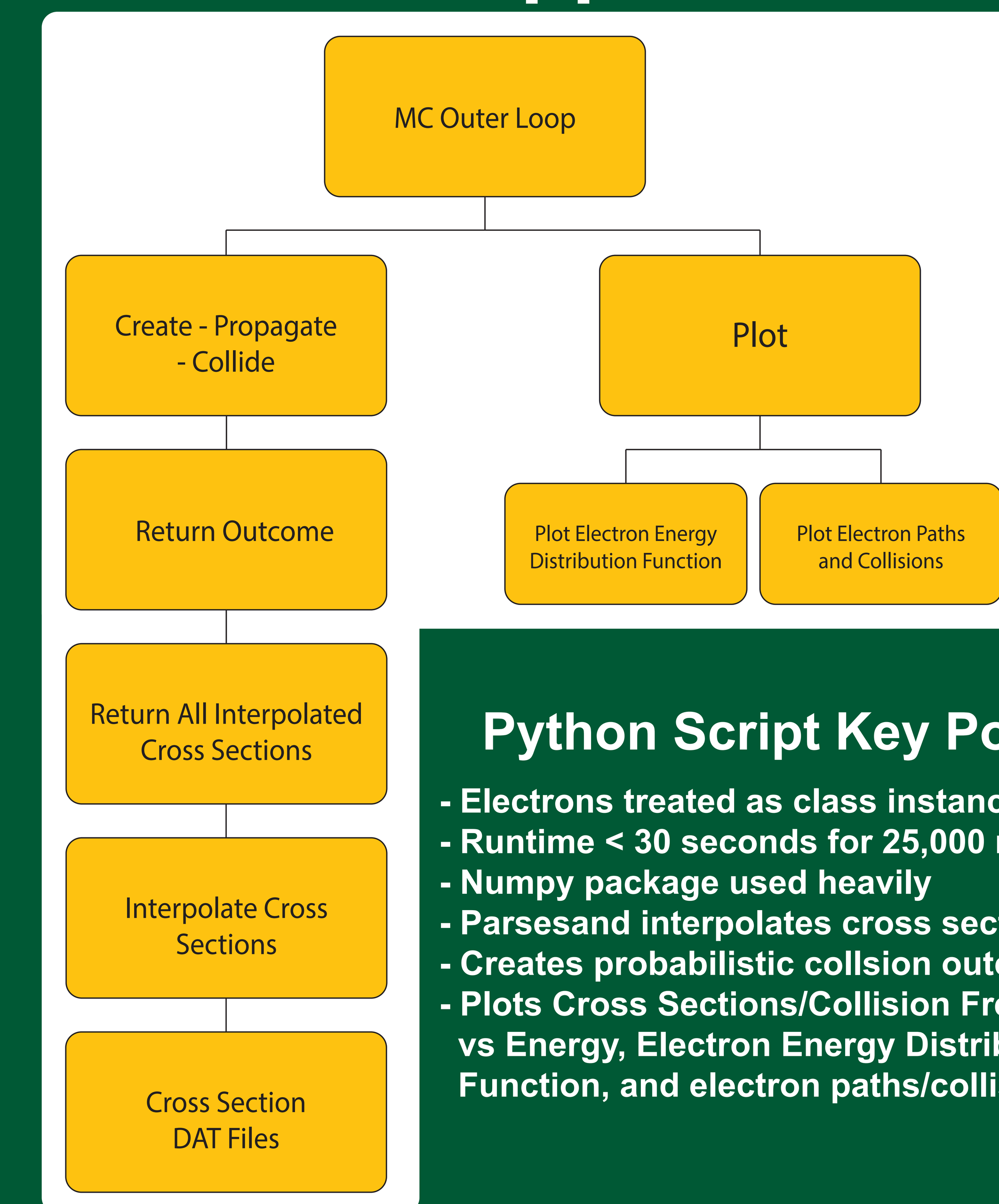
$$v_{fx} = v_{ix} - \frac{m_a}{m_e}v_{ax} \qquad v_{fy} = v_{ix} - \frac{m_a}{m_e}v_{ax}\tan\alpha$$

- ΔE is the energy lost from ionization of excitation
- ά is the electrons scattting angle relative to the positive x-axis
- θ is the electrons incident angle
- γ is the electrons scattting angle relative to the incident path





Code/Approach



Python Script Key Points

- Electrons treated as class instances
- Runtime < 30 seconds for 25,000 motions
- Numpy package used heavily
- Parsesand interpolates cross sections
- Creates probabilistic collsion outcome
- Plots Cross Sections/Collision Frequency vs Energy, Electron Energy Distribution Function, and electron paths/collisions

Results

Initial Conditions/Constraints

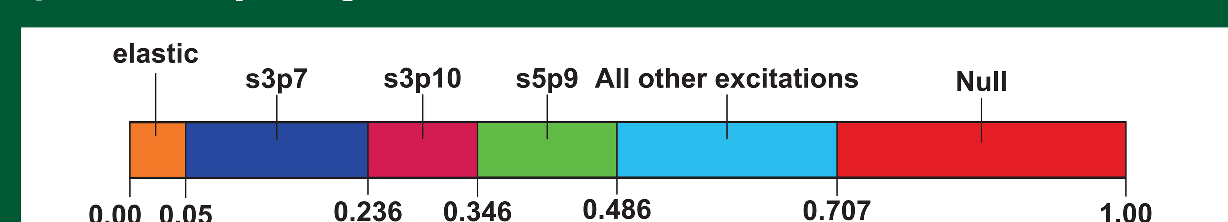
- Population Density NA=10^{21}atoms/cm^3
- 500 electrons propagated 50 times each
- Maximum electron energy of 100 eV
- Trials run for solely horizontal electric field
  - Ex = 5 V/m, Ey= 0 V/m
  - Ex = 25 V/m, Ey= 0 V/m
  - Ex = 50 V/m, Ey= 0 V/m

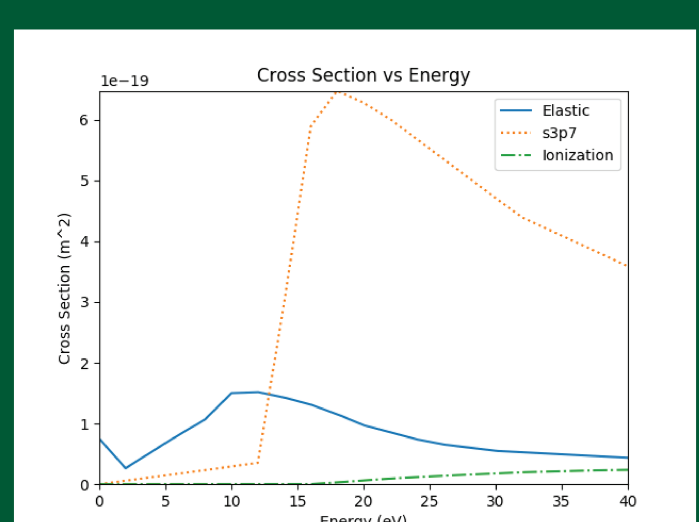
Binning

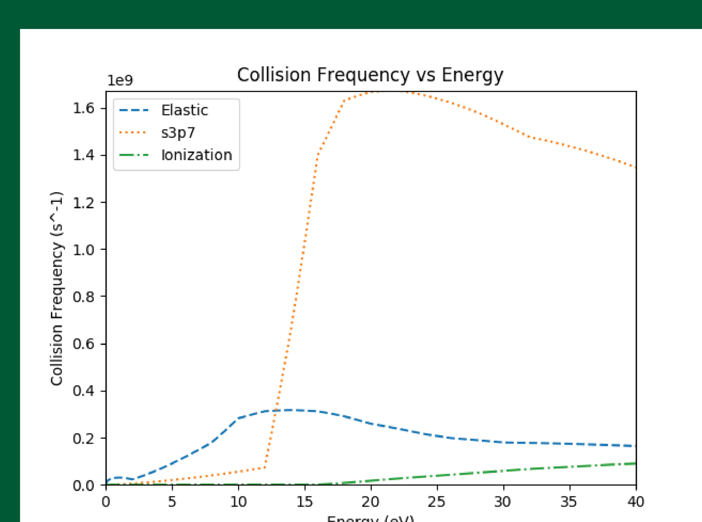
- Script parses through list of all energies experienced at any point
- Creates bins in intervals of 1 electron volt
- Maximum electron energy of 100 eV

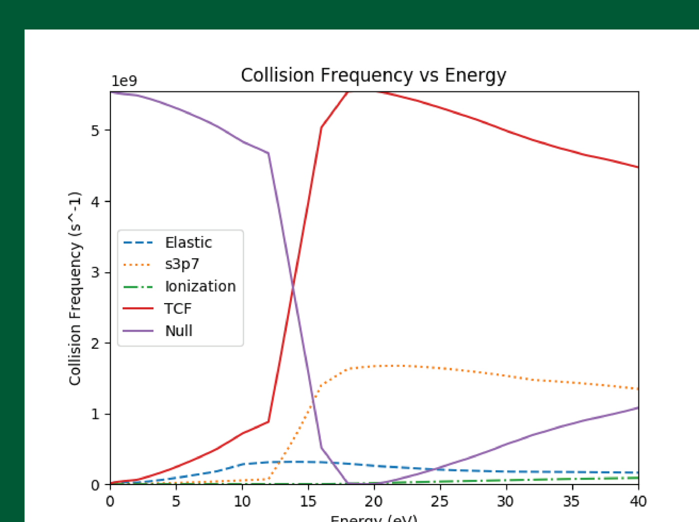
Calculating Probabilities from Collision Frequencies

- Experimentally-measured cross sections give collision frequencies
- Highest cross section s3p7 below as compared with elastic, ionization, TCF as well as NCF for corresponding cross sections and collision frequencies
- Collision frequencies at a given energy scaled by Max TCF
- As seen in graphs below, electrons probabaility to experience null collision, elastic or inelastic collsions depend on their current energy
- Figure below demonstrates collision probabilities at 15 eV
- Python script generates random float between 0 and 1 to make a probabilitiy weighted outcome









Analysis and Conclusion

Overall Trends

-Electron Energy Distribution Function peaked between 5 - 7 eV
-Fell after 10 - 15 eV depending on the electric field strength.

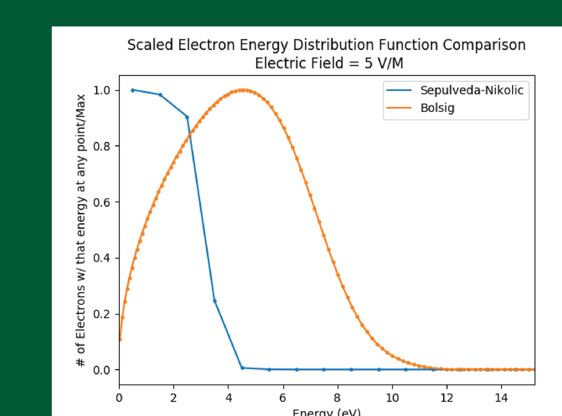
Comparison to previously conducted experiments

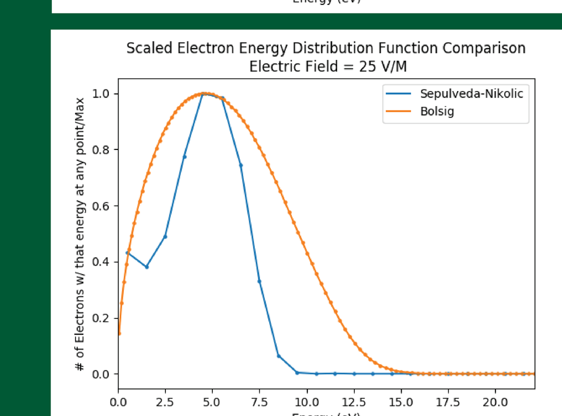
We compared our results with Bolsig and his colleagues who conducted a similar study at three electric field magnitudes andfound that our findings were in good agreement with theirs.
- Scaled finding by maximum bin occurances to accurately compare EEDF's
- In weak electric fields our EEDF trended towards lower energies and started at a peak
- In strong electric fields our EEDF shifted towards slightly higher energies with narrower peak

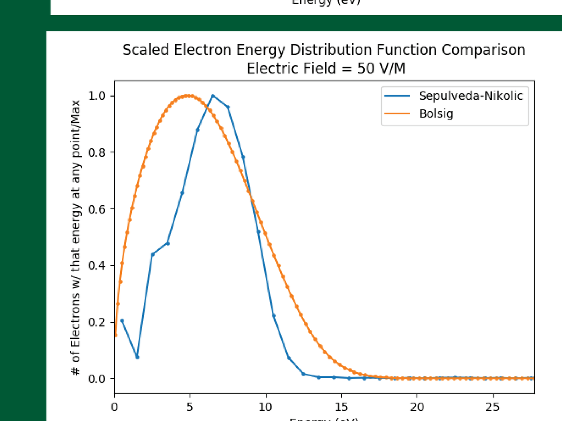
Applications and Areas for Improvement

By continuing to study these properties of plasma, we are able to possibly improve the plasma etching process.This research is ongoing and next steps include but are not limited to

- Taking the simulation from two dimensions to three,
- Improve code efficiency and runtime
- Reduce margins or error







References

[1] G. J. M. Hagelaar and L. C. Pitchford, Plasma Sources Sci. Technol. 14, 722 (2005).
[2] J. Boffard, R. O. Jung, C. C. Lin, and A. E. Wendt, Plasma Sources Sci. Technol. 19, 065001 (2010).